

Claims

We claim:

1. A method of measuring the molecular mass of a compound Y of unknown molecular mass by mass spectrometry, comprising
providing a sample of compound Y,
providing samples of at least two different compounds each of Formula (I), R-X in which R is a trityl group and X is cleavable to form a charged species for mass spectrometry,
and recording the molecular mass of compound Y and the at least two compounds of Formula (I) in a mass spectrometer.
2. The method, according to claim 1, in which R is $R^1R^2R^3C-$ wherein R^1 , R^2 and R^3 are the same or different and each is a monocyclic or fused ring aromatic group that is substituted or unsubstituted.
3. The method, according to claim 2, in which at least one of R^1 , R^2 and R^3 carries a substituent selected from the group consisting of substituted or unsubstituted C_1 - C_{20} alkoxy and hydrocarbyl.
4. The method, according to claim 3, in which the alkoxy or hydrocarbyl is substituted by a substituent selected from the group consisting of carboxylic acid, sulphonic acid, nitro, cyano, hydroxyl, thiol, primary, secondary or tertiary amino, primary or secondary amido, anhydride, carbonyl halide and active ester.
5. The method, according to any of claim 2, in which each of R^1 , R^2 and R^3 is aryl.
6. The method, according to claim 5, wherein said aryl is phenyl.

7. The method, according to claim 1, in which the trityl group R has at least two amide substituents.

8. The method, according to claim 7, wherein said trityl group R has at least four amide substituents.

9. The method, according claim 2, in which R^1 , R^2 and R^3 together carry at least two amide groups and/or at least two reactive groups for coupling.

10. The method, according to claim 9, wherein said groups are N-hydroxy succinimide ester groups.

11. The method, according to claim 1, in which X is halide or tosylate.

12. The method, according to claim 1, comprising providing at least five compounds of Formula (I) and recording their molecular masses in a mass spectrometer.

13. The method, according claim 1, in which the group X is photocleavable to form a charged species for mass spectrometry.

14. The method, according to claim 1, additionally comprising estimating the molecular mass of unknown compound Y as M_y and providing at least one compound of Formula (I) which has known molecular mass M_1 below M_y and at least one different compound of Formula (I) which has molecular mass M_2 above M_y .

15. The method, according to claim 14, wherein the difference between M_y and each of M_1 and M_2 is not more than $\pm 50\%$.

16. The method, according to claim 1, additionally comprising providing a sample of at least one further compound Z of unknown molecular mass and measuring the molecular mass of compound Z.

17. Use of a compound of Formula (I) R-X in which R is a trityl group and X is cleavable to form a charged species for mass spectrometry as a calibration compound for mass spectrometry.

18. A kit for the production of calibration compounds for mass spectrometry comprising:

(a) at least one base reactant of Formula (I) R-X where R is a trityl group and X is cleavable to form a charged species for mass spectrometry; and

(b) at least two different amine compounds which are of different molecular masses and which are each capable of reacting with the base reactant;

wherein the base reactant (a) is packaged separately from amine compounds (b).

19. The kit, according to claim 18, additionally comprising instructions to select at least two desired molecular masses M_1 and M_2 for the calibration compounds and to choose one or more amines for reaction with the base reactant so as to obtain compounds of the desired predetermined molecular masses M_1 and M_2 , and instructions to use the compounds in mass spectrometry.

20. A set of calibration compounds for mass spectrometry comprising at least two separately packaged mixtures (a) and (b), wherein

mixture (a) comprises at least two different compounds each of formula (I) R-X and having different molecular masses, and

mixture (b) comprises at least two further compounds of formula (I) R-X having different molecular masses and wherein R is a trityl group and X is cleavable to form a charged species for mass spectrometry.

21. The set, according to claim 20, in which the lowest molecular mass in mixture (a) is lower than the lowest molecular mass in mixture (b) and the highest molecular mass in mixture (a) is lower than the highest molecular mass in mixture (b).

22. The set, according to claim 20, in which each of mixtures (a) and (b) contains at least five different compounds of different molecular masses.

23. The set, according to claim 22, in which each of mixtures (a) and (b) contains at least 10 different compounds of different molecular masses.

24. The set, according to claim 20, comprising at least three separately packaged mixtures of compounds.

25. The set, according to claim 24, comprising at least five separately packaged mixtures of compounds.

26. A kit for the production of a set of calibration compounds comprising a first package comprising a base reactant of Formula (I) R-X, in which R is a trityl group and X is cleavable to form a charged species for mass spectrometry, and at least two separate second packages (a) and (b), each containing a mixture of at least two amine compounds which have different molecular masses and which are capable of reacting with the base reactant.

27. The kit, according to claim 26, in which the lowest molecular mass in mixture (a) is lower than the lowest molecular mass in mixture (b) and the highest molecular mass in mixture (a) is lower than the highest molecular mass in mixture (b).

28. The kit, according to claim 26, in which each of mixtures (a) and (b) contain at least five different amine compounds of different molecular masses.

29. The kit, according to claim 28, wherein each of mixtures (a) and (b) contain at least ten different amine compounds of molecular masses.

30. The kit, according to claim 26, comprising at least three mixtures of amine compounds.

31. The kit, according to claim 30, comprising at least five mixtures of amine compounds.

32. A method of measuring the molecular mass of a compound Y of unknown molecular mass comprising

estimating the expected molecular mass of compound Y, selecting at least one calibration compound of Formula (I) R-X having molecular weight close to the expected molecular weight of the compound Y, in which R is a trityl group and X is cleavable to form a charged species for mass spectrometry

and subjecting both compounds to mass spectrometry simultaneously.

33. The method, according to claim 32, in which the calibration compound R-X is provided by selecting a base reactant R-X and selecting an amine reactant of appropriate molecular mass and reacting the amine reactant and the base reactant.

34. A mixture of at least two compounds of Formula (I) R-X in which R is a trityl group and X is a group cleavable to give a charged species for analysis by mass spectrometry.

35. The mixture, according to claim 34, comprising at least five different compounds of Formula (I).

36. The mixture, according to claim 35, comprising at least ten different compounds of Formula (I).

37. A method of mass spectrometry comprising subjecting simultaneously to mass spectrometry at least two different compounds of Formula (I) R-X in which R is a trityl group and X is cleavable to give a charged species for analysis by mass spectrometry.